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LOGINID:ssspta1621con

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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Welcome to STN International
                 Web Page for STN Seminar Schedule - N. America
NEWS
         OCT 02
                 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
NEWS
        OCT 19
                 BEILSTEIN updated with new compounds
        NOV 15
NEWS
                 Derwent Indian patent publication number format enhanced
                 WPIX enhanced with XML display format
        NOV 19
NEWS
        NOV 30
NEWS
                 ICSD reloaded with enhancements
NEWS
         DEC 04
                 LINPADOCDB now available on STN
NEWS 8
         DEC 14
                 BEILSTEIN pricing structure to change
        DEC 17
NEWS 9
                 USPATOLD added to additional database clusters
NEWS 10
        DEC 17
                 IMSDRUGCONF removed from database clusters and STN
         DEC 17
NEWS 11
                 DGENE now includes more than 10 million sequences
         DEC 17
                 TOXCENTER enhanced with 2008 MeSH vocabulary in
NEWS 12
                 MEDLINE segment
         DEC 17
                 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 13
NEWS 14
         DEC 17
                 CA/CAplus enhanced with new custom IPC display formats
         DEC 17
NEWS 15
                 STN Viewer enhanced with full-text patent content
                 from USPATOLD
NEWS 16
         JAN 02
                 STN pricing information for 2008 now available
NEWS 17
                 CAS patent coverage enhanced to include exemplified
         JAN 16
                 prophetic substances
         JAN 28
                 USPATFULL, USPAT2, and USPATOLD enhanced with new
NEWS 18
                 custom IPC display formats
NEWS 19
         JAN 28
                 MARPAT searching enhanced
NEWS 20
         JAN 28
                 USGENE now provides USPTO sequence data within 3 days
                 of publication
NEWS 21
         JAN 28
                 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22
         JAN 28
                 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23
         FEB 08
                 STN Express, Version 8.3, now available
NEWS 24
         FEB 20
                 PCI now available as a replacement to DPCI
NEWS 25 .
         FEB 25
                 IFIREF reloaded with enhancements
NEWS 26
         FEB 25
                 IMSPRODUCT reloaded with enhancements
NEWS 27
         FEB 29
                 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                 U.S. National Patent Classification
NEWS 28
         FEB 31
                 IFICDB, IFIPAT, and IFIUDB enhanced with new custom
                 IPC display formats
NEWS 29
         FEB 31
                 CAS REGISTRY enhanced with additional experimental
                 spectra
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NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

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NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 08:16:56 ON 31 MAR 2008

=> FILE CSAREACT

'CSAREACT' IS NOT A VALID FILE NAME SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> FILE CASREACT COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 08:17:56 ON 31 MAR 2008 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE CONTENT:1840 - 29 Mar 2008 VOL 148 ISS 14

New CAS Information Use Policies, enter HELP USAGETERMS for details.

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Uploading C:\Program Files\Stnexp\Queries\APP-102.str

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chain nodes :
13  14  15  16  17  18  19  20  21  22  23  24  25  26  27  28  29  36  37  38  39  40  41  42  43  44
ring nodes :
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ring bonds :
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31-32 32-33 33-34 34-35
exact/norm bonds :
7-8 7-12 8-9 9-10 10-11 10-13 11-12 12-14 15-16 36-40
exact bonds :
1-21 2-22 3-15 4-17 5-20 6-18 7-23 7-24 8-25 8-26 9-27 9-28 11-15
11-29 18-19 30-37 31-44 32-43 33-36 34-38 35-42 36-39 37-41
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 30-31 \quad 30-35 \quad 31-32 \quad 32-33 \quad 33-34 \quad 34-35
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Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS fragments assigned product role: containing 1 fragments assigned reactant/reagent role: containing 30 L1STRUCTURE UPLOADED => S L1 FULL FULL SEARCH INITIATED 08:19:43 FILE 'CASREACT' SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 2 DOCUMENTS 100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS SEARCH TIME: 00.00.01 O SEA SSS FUL L1 (O REACTIONS) L2 Uploading C:\Program Files\Stnexp\Queries\APP-102.str product STRUCTURE UPLOADED Uploading C:\Program Files\Stnexp\Queries\APP-102.str reactant/reagent => S L3 FULL FULL SEARCH INITIATED 08:20:42 FILE 'CASREACT' SCREENING COMPLETE - 72 REACTIONS TO VERIFY FROM 12 DOCUMENTS 72 VERIFIED 3 HIT RXNS 100.0% DONE 1 DOCS SEARCH TIME: 00.00.01 1 SEA SSS FUL L3 (3 REACTIONS) => D L4 IBIB ABS CRD 1 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 131:31801 CASREACT TITLE: Preparation of acylated cyclic 1,3-dicarbonyl compounds by rearrangement of enol esters INVENTOR(S): Brown, Stephen Martin; Bentley, Thomas William; Jones, Robert Oliver PATENT ASSIGNEE(S): Zeneca Limited, UK PCT Int. Appl., 23 pp. SOURCE: CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

APPLICATION NO. DATE

KIND DATE

PATENT NO.

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WO 9928282
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PRIORITY APPLN. INFO.:
                                            WO 1998-GB3458
                                                              19981117
```

OTHER SOURCE(S): MARPAT 131:31801

GI For diagram(s), see printed CA Issue.

The title compds. [I; R = (un) substituted Ph, (un) substituted C3-6 cycloalkyl; Q = (un) substituted 5- or 6-membered saturated carbocyclic ring], especially benzoyl- and cycloalkyl-1,3-cyclohexanediones useful as herbicides and plant growth regulators (no data), were prepared by rearrangement of enol esters (II; Q, R as defined) in a (di)polar aprotic or aromatic hydrocarbon solvent in the presence of a moderate base and an azole instead of a cyanide catalyst. For example, stirring a mixture of 2.31 g 1,3-cyclohexanedione, 1.5 g K2CO3 and 20 mL MeCN for 3 h at 35°, adding 1.5 g PhCOCl and stirring for 30 min, adding 2 g K2CO3 and 0.035 g 1,2,4-triazole and stirring the whole for 16 h at 25° gave 2-benzoyl-1,3-cyclohexanedione in 90% yield.

RX(2) OF 10

RX(6) OF 10

NOTE: phase-transfer conditions are claimed

RX(10) OF 10 - 2 STEPS

1.1. PhMe, DMF

1.2. SOC12, PhMe 1.3. 1,2,4-Triazole, PhMe

2.1. K2CO3, MeCN

2.2. HCl, Water

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

---Logging off of STN---

Executing the logoff script...

-=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	${ t TOTAL}$
	ENTRY	SESSION
FULL ESTIMATED COST	244.69	245.11
•		
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

STN INTERNATIONAL LOGOFF AT 08:22:32 ON 31 MAR 2008

6



Connecting via Winsock to STN

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PASSWORD:

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NEWS
                 Web Page for STN Seminar Schedule - N. America
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         OCT 02
                 CA/CAplus enhanced with pre-1907 records from Chemisches
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NEWS
         OCT 19
                 BEILSTEIN updated with new compounds
NEWS
         NOV 15
                 Derwent Indian patent publication number format enhanced
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         NOV 19
NEWS
         NOV 30
                 ICSD reloaded with enhancements
NEWS
         DEC 04
                 LINPADOCDB now available on STN
         DEC 14
                 BEILSTEIN pricing structure to change
NEWS
NEWS
        DEC 17
                 USPATOLD added to additional database clusters
         DEC 17
NEWS 10
                 IMSDRUGCONF removed from database clusters and STN
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NEWS 11
                 DGENE now includes more than 10 million sequences
NEWS 12
         DEC 17
                 TOXCENTER enhanced with 2008 MeSH vocabulary in
                 MEDLINE segment
         DEC 17
NEWS 13
                 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14
         DEC 17
                 CA/CAplus enhanced with new custom IPC display formats
         DEC 17
NEWS 15
                 STN Viewer enhanced with full-text patent content
                 from USPATOLD
NEWS 16
         JAN 02
                 STN pricing information for 2008 now available
NEWS 17
         JAN 16
                 CAS patent coverage enhanced to include exemplified
                 prophetic substances
NEWS 18
         JAN 28
                 USPATFULL, USPAT2, and USPATOLD enhanced with new
                 custom IPC display formats
NEWS 19
         JAN 28
                 MARPAT searching enhanced
NEWS 20
         JAN 28
                 USGENE now provides USPTO sequence data within 3 days
                 of publication
NEWS 21
         JAN 28
                 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22
         JAN 28
                 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23
         FEB 08
                 STN Express, Version 8.3, now available
NEWS 24
         FEB 20
                 PCI now available as a replacement to DPCI
NEWS 25
         FEB 25
                 IFIREF reloaded with enhancements
NEWS 26
         FEB 25
                 IMSPRODUCT reloaded with enhancements
NEWS 27
         FEB 29
                 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                 U.S. National Patent Classification
NEWS 28
         FEB 31
                 IFICDB, IFIPAT, and IFIUDB enhanced with new custom
                 IPC display formats
NEWS 29
         FEB 31
                 CAS REGISTRY enhanced with additional experimental
                 spectra
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NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

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=> FILE CASREACT COST IN U.S. DOLLARS

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SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

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FILE CONTENT: 1840 - 29 Mar 2008 VOL 148 ISS 14

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This file contains CAS Registry Numbers for easy and accurate substance identification.

Uploading C:\Program Files\Stnexp\Queries\APP-121.str

chain nodes :
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ring nodes :
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chain bonds :
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13-15 16-17 16-18 21-24 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
16-18
exact bonds :
1-21 2-30 3-29 4-16 5-20 6-28 7-22 8-27 9-26 10-13 11-19 12-25 16-17
21-24 22-23
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-15

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS fragments assigned product role: containing 1 fragments assigned reactant/reagent role: containing 7 L1STRUCTURE UPLOADED => S L1 FULL FULL SEARCH INITIATED 08:50:47 FILE 'CASREACT' SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS 100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS SEARCH TIME: 00.00.01 L2 O SEA SSS FUL L1 (O REACTIONS) Uploading C:\Program Files\Stnexp\Queries\APP-121.str product L3 STRUCTURE UPLOADED Uploading C:\Program Files\Stnexp\Queries\APP-121.str reactant/reagent STRUCTURE UPLOADED => S L4 FULL FULL SEARCH INITIATED 08:51:54 FILE 'CASREACT' SCREENING COMPLETE - 60 REACTIONS TO VERIFY FROM 11 DOCUMENTS 60 VERIFIED 100.0% DONE 9 HIT RXNS 6 DOCS SEARCH TIME: 00.00.01 L5 6 SEA SSS FUL L4 (9 REACTIONS) => D L5 IBIB ABS CRD 1-6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 144:88169 CASREACT TITLE: Process for the preparation of substituted bicyclooctenes and their use as herbicides INVENTOR(S): Beaudegnies, Renaud; Luethy, Christoph; Edmunds, Andrew; Schaetzer, Juergen; Wendeborn, Sebastian PATENT ASSIGNEE(S): Syngenta Participations AG, Switz. SOURCE: PCT Int. Appl., 109 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2005123667 A1 20051229 WO 2005-EP6707 20050621

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

APPLN. INFO::

CH 2004-1050 20040622
```

PRIORITY APPLN. INFO.:

CH 2004-1050 20040022 CH 2004-1051 20040622

OTHER SOURCE(S):

MARPAT 144:88169

GI

Compds. I [A1 = N, CR7, A2 = N, CR8; R1, R2, R7, R8 = H, C1-6-alkyl,AB C2-6-alkenyl, C2-6-alkynyl, halogen, OH, SH, NO2, CN, (C1-6alkoxy)carbonyl, (C1-6-alkyl)carbonyl, CHO, CH:NOH, (C1-6alkoxy)iminomethylene, C1-6-alkoxy, C1-6-haloalkoxy, C3-6-alkenyloxy, C3-6-alkynyloxy, (C1-4-alkoxy)-(C1-2-alkoxy), (C1-6-alkoxy)carbonyloxy, C1-6-alkylthio, C1-6-alkylsulfonyl, C1-6-alkylsulfinyl, etc.; R3 = OH, O-M+, halogen, C1-8-alkoxy, SH, C1-8-alkylthio, C1-8-alkylsulfinyl, C1-8-alkylsulfonyl, C1-8-haloalkylthio, C1-8-haloalkylsulfinyl, C1-8-haloalkylsulfonyl, (C1-4-alkoxy)-(C1-4-alkyl)thio, (C1-4-alkoxy)-(C1-4-alkyl) sulfinyl, (C1-4-alkoxy)-(C1-4-alkyl) sulfonyl, (C3-8-alkenyl)thio, (C3-8-alkynyl)thio, (C1-4-alkylthio)-(C1-4-alkyl)thio, (C3-4-alkenyl)thio-(C1-4-alkyl)thio, (C1-4-alkoxy)carbonyl-(C1-4alkyl)thio, (C1-4-alkoxy)carbonyl-(C1-4-alkyl)sulfinyl,(C1-4alkoxy)carbonyl-(C1-4-alkyl)sulfonyl,etc.; M+ = alkali metal ion, ammonium cation; Q = Ph (optionally substituted with up to 4 substituents); Y = O, NR4a, S, S(:O), SO2, C(:O), C(:NR4b), C(:CR6aR6b), C1-4-alkylene, C2-4-alkenylene; R4a = ; R4b = ; R6a = H, C1-6-alkyl, (C1-6-alkyl)alkyl)carbonyl, (C1-6-alkyl)carbonyloxy; R6b = H, C1-6-alkyl; R6aR6b = C2-5-alkylene] are suitable for use as herbicides. The process for the preparation of substituted bicyclooctenes comprises: (a) converting cyclopropane II [Xa = H, Cl, Br, I; Xb, Xc, Xd = halogen; Za = halogen, C1-6-alkoxy, OPh, C1-6-alkylthio, C1-6-alkylsulfinyl, C1-6-alkylsulfonyl, SPh, S(:0)Ph, SO2Ph] in an anhydrous inert solvent containing an alkali metal hydroxide to cyclopropene III; (b) reacting III with cyclopentadiene IV; and (c) hydrolysis in the presence of an aqueous base. Thus, 3-[4-(Methanesulfonyl)-2-nitrobenzoyl]bicyclo[3.2.1]oct-6-ene-2,4-dione [I; A1 = A2 = CH, Q = C6H4NO2-2-(SO2Me)-4, R1 = R2 = H, R3 = OH, Y = CH2] was prepared from cyclopentadiene via cycloaddn. with

pentachlorocyclopropane in dioxane containing KOH, hydrolysis with aqueous NaOH.

reduction with Zn in AcOH, and acylation with 4-(methanesulfonyl)-2nitrobenzoic acid in MeCN containing dicyclohexylcarbodiimide in CH2Cl2, Et3N and acetone cyanohydrin. The pre- and post-emergence herbicidal activity of I [A1 = A2 = CH, Q = C6H4NO2-2-(SO2Me)-4, R1 = R2 = H, R3 = OH, Y = CH2; (at 250 g/ha)] was determined [pre-emergence: total damage = 9/10 vs. Panicum; total damage = 9/10 vs. Echinochloa; total damage = 9/10 vs. Amaranthus; total damage = 9/10 vs. Sinapis; total damage = 9/10 vs. Stellaria; post-emergence: total damage = 7/10 vs. Echinochloa; total damage = /10 vs. Xanthium; total damage = 9/10 vs. Ipomea; total damage = 10/10 vs. Chenopodium; total damage = 9/10 vs. Kochia; total damage = 9/10 vs. Sinapis; total damage = 9/10 vs. Stellaria].

CON: STAGE(1) room temperature

STAGE(2) 2.5 hours, room temperature

STAGE(3) room temperature STAGE(4) 18 hours, room temperature

STAGE(5) room temperature, pH 1

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

143:459878 CASREACT

TITLE:

SOURCE:

Multi-step process for the production of cyclic

diketones

INVENTOR(S):

Jackson, David Anthony; Edmunds, Andrew; Bowden,

Martin Charles; Brockbank, Ben

PATENT ASSIGNEE(S):

Syngenta Participations AG, Switz.; Syngenta Limited

PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PA	rent	NO.		KI	ND	DATE			Α	PPLI	CATI	N NC	ο.	DATE			
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
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														MW,			

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PRIORITY APPLN. INFO.:
                                            CH 2004-765
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OTHER SOURCE(S): MARPAT 143:459878

AB A multi-step process for the preparation of cyclic diketones [e.g., 4-(4-chlorophenylcarbonyloxy)bicyclo[3.2.1]oct-3-en-2-one] is presented.

RX(10) OF 15

CON: STAGE(1) 15 minutes, room temperature; 18 hours, 45 deg C; 45 deg C -> reflux; 40 hours, reflux

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS 'RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

143:459877 CASREACT

TITLE: INVENTOR(S):

Process for the production of cyclic diketones Jackson, David Anthony; Edmunds, Andrew; Bowden,

Martin Charles; Brockbank, Ben

PATENT ASSIGNEE(S):

Syngenta Participations A.-G., Switz.; Syngenta

Limited

SOURCE:

PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE: E FAMILY ACC. NUM. COUNT: 1

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APPLICATION NO.
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PRIORITY APPLN. INFO.:
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OTHER SOURCE(S): MARPAT 143:459877

A process for the preparation of cyclic diketones [e.g., 4-(4chlorophenylcarbonyloxy)bicyclo[3.2.1]oct-3-en-2-one] is presented.

Me S
$$CO_2H$$
 + $C1$ $EtN(Pr-i)2, ZnC12, MeCN$

CON: STAGE(1) 15 minutes, room temperature; room temperature -> 45 deg C; 18 hours, 45 deg C; 45 deg C -> reflux; 40 hours, reflux

ANSWER 4 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:42165 CASREACT

TITLE: Acylation of cyclic 1,3-diketones with Ph esters in the presence of cyanide or fluoride ion.

INVENTOR(S): Wojtkowski, Paul Walter PATENT ASSIGNEE(S):

E.I. Du Pont de Nemours and Co., USA

SOURCE:

U.S. Pat. Appl. Publ., 19 pp., Cont.-in-part of U.S.

Ser. No. 833,451, abandoned.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030232984	A1	20031218	US 2003-396047	20030324
US 6809206	B2	20041026		
US 20020049317	A1	20020425	US 2001-833451	20010412
PRIORITY APPLN. INFO.	:		US 1999-120213P	19990212
			US 2000-483644	20000114
			US 2001-833451	20010412

OTHER SOURCE(S):

MARPAT 140:42165

GΙ

AB Title compds. [I; A = linker comprising 2-4 C, 0-2 N, 0-2 O, and 0-2 S atoms; J = (substituted) C-linked hydrocarbyl; Y = H, salt cation], were prepared by treatment of the corresponding diketones with RyC6H5-yO2CJ (R = electron withdrawing group; y = 0-3; J as above) in the presence of CN- or F-. Thus, 2-(methoxycarbonyl)phenyl 2,3-dihydro-5,8-dimethylspiro(4H-1benzothiopyran-4,2'-[1,3]dioxolane)-6-carboxylate 1,1-dioxide (preparation given), 1,3-cyclohexanedione, Et3N, and KCN were heated in MeCN in a sealed tube for 10 h at 90° to give 2-[[2,3-dihydro-5,8-dimethyl-1,1-dioxidospiro(4H-1-benzothiopyran-4,2'-[1,3]dioxolan)-6-yl]carbonyl]-3hydroxy-2-cyclohexen-1-one Et3N salt.

CON: STAGE(1) room temperature; 1 hour, room temperature STAGE(2) room temperature; 1 hour, room temperature

RX(30) OF 31 - 2 STEPS

1.1. DMF, (COC1)2, CH2C12

1.2. 4-02NC6H4OH, Et3N, CH2Cl2 2.1. Me2C(OH)CN, Et3N,

MeCN 2.2. NaHCO3, Water

CON: STEP(1.1) room temperature; 1 hour, room temperature STEP(1.2) room temperature; 1 hour, room temperature STEP(2) 1 hour, 22 deg C

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

136:340425 CASREACT

TITLE:

Method for acylating cyclic 1,3-diketones with phenyl

ester derivatives to yield triketones

INVENTOR(S):

Wojtkowski, Paul Walter

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S. Pat. Appl. Publ., 20 pp., Cont.-in-part of U.S.

Ser. No. 483,644.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

•	PATENT NO.	KIND	DATE	API	PLICATION NO.	DATE
	US 20020049317	A1	20020425	US	2001-833451	20010412
	US 20030232984	A1	20031218	US	2003-396047	20030324
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PRIO	RITY APPLN. INFO.	:		US	2000-483644	20000114
				US	1999-120213P	19990212
				US	2001-833451	20010412

OTHER SOURCE(S):

MARPAT 136:340425

GΙ

AB A method is disclosed for the preparation of I by acylation of II with Ar-OCOJ in the presence of a cyanide or fluoride catalyst [A = linking group comprising an (un)substituted backbone segment consisting of 2 to 4 atoms selected from carbon atoms and 0-2 N, O, or S atoms; J = (un)substituted, carbon-linked hydrocarbyl group; Y = H or a salt cation; Ar = (un)substituted phenyl]. Forty-one examples are provided. For instance, 2-[2-chloro-4-(methylsulfonyl)benzoyl]-3-hydroxy-2-cyclohexen-1-one (III) was prepared from 4-nitrophenyl 2-chloro-4-(methylsulfonyl)benzoate (preparation

given) and 1,3-cyclohexanedione in the presence of acetone cyanohydrin and triethylamine in acetonitrile for 3 h at 22°C. Ph ester substitution and sources of cyanide and fluoride were evaluated in the examples. Utilization of Ph esters as acylation agents worked well in the one step process and can be prepared under mild, acid-free conditions preserving sensitive functionality vulnerable to degradation under reaction conditions used to prepare acyl chlorides of prior art processes.

RX(27) OF 28 - 2 STEPS

ANSWER 6 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

131:31801 CASREACT

TITLE:

Preparation of acylated cyclic 1,3-dicarbonyl

compounds by rearrangement of enol esters

INVENTOR(S):

Brown, Stephen Martin; Bentley, Thomas William; Jones,

Robert Oliver

PATENT ASSIGNEE(S):

Zeneca Limited, UK

SOURCE:

PCT Int. Appl., 23 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PAT	TENT	NO.		KI	ΝD	DATE			А	PPLI	CATI	ON NO	Э.	DATE			
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PRIORITY APPLN. INFO.:
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OTHER SOURCE(S): MARPAT 131:31801

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R = (un)substituted Ph, (un)substituted C3-6 cycloalkyl; Q = (un)substituted 5- or 6-membered saturated carbocyclic ring], especially benzoyl- and cycloalkyl-1,3-cyclohexanediones useful as herbicides and plant growth regulators (no data), were prepared by rearrangement of enol esters (II; Q, R as defined) in a (di)polar aprotic or aromatic hydrocarbon solvent in the presence of a moderate base and an azole instead of a cyanide catalyst. For example, stirring a mixture of 2.31 g 1,3-cyclohexanedione, 1.5 g K2CO3 and 20 mL MeCN for 3 h at 35°, adding 1.5 g PhCOCl and stirring for 30 min, adding 2 g K2CO3 and 0.035 g 1,2,4-triazole and stirring the whole for 16 h at 25° gave 2-benzoyl-1,3-cyclohexanedione in 90% yield.

RX(10) OF 10 - 2 STEPS

6

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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